Electron Impact Ionization Cross Sections and Rate Coefficients for the CS_2 Molecule

Neeraj Kumar[†]

Department of Physics, D.A.V. College, Muzaffarnagar, Uttar Pradesh, 251001, INDIA

The electron impact ionization cross section of carbon disulfide (CS_2) molecule has been evaluated systematically by using the semi-empirical Jain-Khare formalism. This approach combines quantum mechanical ideas with empirical corrections to predict ionization cross sections accurately, particularly for complex polyatomic molecules. In the present work, total ionization cross sections have been calculated over a range of incident electron energies from the ionization threshold to 1000 eV, incorporating molecular parameters such as the ionization potential, the distribution of oscillator strength, and the number of active electrons into the Jain-Khare formalism [1]. The partial ionization cross sections for the production of the main fragment ions—CS_2^+, CS^+, S_2^+, and S^+ were also obtained by incorporating appearance energies and relative yields into the model.

The results show a sharp onset of ionization cross sections at the threshold. At this threshold, the cross section rises sharply, reaching a maximum value at higher energies before gradually decreasing as the electron energy continues to increase. This trend is typical for polyatomic molecules. The agreement with experimental data [2-5] and other theoretical models [5-7] proves the accuracy and versatility of the Jain-Khare approach for total as well as fragment-specific ionization processes. These results are essential for validating models and simulating electron-driven processes in environments such as plasmas and planetary atmospheres where CS_2 is present. In addition to the evaluation of ionization cross sections, we have also calculated the ionization rate coefficients corresponding to the produced cations using the evaluated ionization cross sections and the Maxwell-Boltzmann distribution as a function of electron temperature/energy. Instead of cross sections themselves, ionization rate coefficients are more important in various plasma applications, gas discharge, and flowing after glow studies [8–9].

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[†]E-mail: drnkumarphy@gmail.com